

Reduced fidelity approach for quantum phase transitions in spin-1/2 dimerized Heisenberg chains

Heng-Na Xiong,¹ Jian Ma,¹ Zhe Sun,² and Xiaoguang Wang^{1,*}

¹*Zhejiang Institute of Modern Physics, Department of Physics,
Zhejiang University, HangZhou 310027, People's Republic of China.*

²*Department of Physics, HangZhou Normal University, HangZhou 310036, People's Republic of China.*

(Dated: February 26, 2009)

We use reduced fidelity approach to characterize quantum phase transitions in the one-dimensional spin-1/2 dimerized Heisenberg chain in the antiferromagnetic case. The reduced fidelity susceptibilities between two nearest-neighboring spin pairs are considered. We find that they are directly related to the square of the second derivative of the ground-state energy. This enables us to conclude that the former might be a more effective indicator of the second-order quantum phase transitions than the latter. Two further exemplifications are given to confirm the conclusion is available for a broad class of systems with SU(2) and translation symmetries. Moreover, a general connection between reduced fidelity susceptibility and quantum phase transitions is illustrated.

PACS numbers: 75.10.Pq, 03.67.-a, 75.10.Jm

I. INTRODUCTION

Quantum phase transitions (QPTs) is an essential phenomenon in quantum many-body correlated system. It is induced by the ground-state (GS) transition driven by external parameters at zero temperature. How to characterize QPTs has attracted widespread attention. Conventionally, QPTs are described in terms of order parameter and symmetry breaking within the Landau-Ginzburg paradigm [1]. One object in these traditional ways is that there is no general method to find the order parameter for a common system. To overcome this problem, a concept called *fidelity* [2, 3] (see Eqs. (6) and (7)) is borrowed from the field of quantum-information theory, since it well describes the overlap between two states in different phases with different structural properties, i.e., order parameters. Thus it does not need a priori knowledge of the order parameter in detecting QPTs. It is a purely Hilbert-space geometrical quantity. On the other hand, *fidelity susceptibility* [4, 5] (see Eq. (8)) is found more convenient than fidelity itself for its independence of the slightly changed external parameters. Hitherto, these two connected concepts have succeeded in identifying the QPTs of many systems, such as XY spin chains and Dicke model [3], XXZ chain [6], Hubbard model [7, 8], frustrated Heisenberg chain [9], Kitaev honeycomb model [10], extended Harper model [11]. The intrinsic relation between the GS fidelity (or fidelity susceptibility) and the characterization of a quantum phase transition has been unveiled in Ref. [12]. It was shown that the singularity and scaling behavior of the GS fidelity (or fidelity susceptibility) are directly related to its corresponding derivative of GS energy, which characterizes the QPTs conventionally. Moreover, the fidelity

susceptibility is associated with dynamic structure factor for QPTs and with specific heat and magnetic susceptibility for thermal phase transitions [13].

The above works are all concerned with the global GS fidelity. Then there is a natural question that whether the fidelity of the subsystem, i.e., the *reduced fidelity* (or named *partial-state fidelity*) could reflect the QPTs. Recently, some works have been devoted to this subject. Zhou *et al.* [14] found that it succeeds in capturing non-trivial information along renormalization group flows and in detecting the QPTs in XY model [15]. Paunković *et al.* [16] showed that it enables them to identify the on-site magnetization as the order parameter for the phase transition in the conventional BCS superconductor with an inserted magnetic impurity system. Kwok *et al.* [17] tested its effectiveness in characterizing the QPTs of the isotropic Lipkin-Meshkov-Glick model and the antiferromagnetic one-dimensional Heisenberg model. Meanwhile, we derived a general expression for the two-site reduced fidelity susceptibility (RFS). It has been applied to the study of the Lipkin-Meshkov-Glick model [18] and transverse field Ising model [19]. We found that the RFS shows similar scaling behavior to the global fidelity susceptibility. All the above works illustrate that the reduced fidelity approach is also an effective tool in identifying QPTs. However, a general relation between RFS and QPTs is not established.

In this work, we apply the reduced fidelity approach to the one-dimensional (1D) spin-1/2 Heisenberg chain with dimerization. Thanks to the SU(2) and translation symmetries, we derive general expressions of the two-site RFSs (the RFSs we mentioned below are all for two-site.), which are connected closely to the square of the second derivative of the GS energy. This result indicates that the RFS is an more effective tool to identify the second-order QPTs than the second derivative of the GS energy. To further testify our conclusion, we exemplify the mixed-spin dimerized Heisenberg chain and the spin-1 bilinear-biquadratic model as well. These two models are both

*Electronic address: xgwang@zimp.zju.edu.cn

of SU(2) and translation symmetries too. Furthermore, it is illustrated that, in general, the origin for RFS to signal QPTs may root in the relation between the reduced density matrix (RDM) and the derivatives of GS energy.

This paper is organized as follows. In Sec. II, we derive a general expression of RFS for two Hermitian and semi-positive definite density matrices, which are commute with each other, and give a direct connection between RFSs and QPTs in the dimerized model. In Sec. III, the critical behavior of the system is studied for both finite-size and infinite-size situations. In Sec. IV, two further models are enumerated and a possible origin between the relation of general reduced fidelity and QPTs is illustrated. Finally, a summary is presented in Sec. V.

II. REDUCED FIDELITY SUSCEPTIBILITY AND ITS CONNECTION TO QUANTUM PHASE TRANSITIONS

The dimerized Heisenberg chain is a fundamental spin-correlated model. It is of special interest both in theory and experiment, since it gives a reasonably accurate description of many quasi-1D antiferromagnets which have two important but structurally inequivalent superexchange paths that are spatially linked, such as the materials of $\text{Cu}(\text{NO}_3)_2 \cdot 2.5\text{H}_2\text{O}$, $(\text{VO})_2\text{P}_2\text{O}_7$ and various aromatic free-radical compounds [20]. Therefore, many efforts have been devoted to study its quantum critical behavior of the dimerized Heisenberg model using various methods, e.g., continuous unitary transformations [21], density matrix renormalization group [22], concurrence [23] and block entanglement [24]. Here we employ the reduced fidelity approach to study the QPTs of this model.

The Hamiltonian for antiferromagnetic Heisenberg chain (AHC) with dimerization reads

$$H_D = \sum_{i=1}^{N/2} (\mathbf{S}_{2i-1} \cdot \mathbf{S}_{2i} + \alpha \mathbf{S}_{2i} \cdot \mathbf{S}_{2i+1}), \quad (1)$$

where \mathbf{S}_i denotes the i -th spin-1/2 operator, and $\alpha > 0$ is the ratio between the two kinds nearest-neighboring (NN) couplings. The total number of spins N is required to be even and the periodic boundary condition $\mathbf{S}_1 = \mathbf{S}_{N+1}$ is assumed.

A. Reduced density matrix

To study the RFS, we need to know the RDM between two spins, and through the whole discussion we restrict to the case of two NN spin pairs. The Hamiltonian has the SU(2) symmetry, i.e., $[H, \sum_{i=1}^N S_{i\gamma}] = 0$ ($\gamma = x, y, z$), which guarantees the RDM between two NN spins is of the form [25]

$$\rho_{ij} = \text{diag}(\varrho_1, \varrho_2), \quad (2)$$

with

$$\varrho_1 = \begin{pmatrix} u^+ & 0 \\ 0 & u^+ \end{pmatrix}, \quad \varrho_2 = \begin{pmatrix} u^- & w \\ w & u^- \end{pmatrix}, \quad (3)$$

in the basis $\{|00\rangle, |11\rangle, |01\rangle, |10\rangle\}$, where $\sigma_z|0\rangle = -|0\rangle$ and $\sigma_z|1\rangle = |1\rangle$. The matrix elements are given by [25]

$$\begin{aligned} u^\pm &= \frac{1}{4} (1 \pm \langle \sigma_{iz} \sigma_{jz} \rangle), \\ w &= \frac{1}{2} \langle \sigma_{iz} \sigma_{jz} \rangle. \end{aligned} \quad (4)$$

This implies the RDM ρ_{ij} is only related to the spin correlator $\langle \sigma_{iz} \sigma_{jz} \rangle$. It is noticed that both ϱ_1 and ϱ_2 are Hermitian, and they can be rewritten in terms of Pauli operators as $\varrho_1 = u\mathbf{I}$, $\varrho_2 = w\mathbf{I} + z\sigma_x$, where \mathbf{I} denotes a 2×2 identity matrix. Therefore, it is found that $\varrho_i \equiv \varrho_i(\alpha)$ ($i = 1, 2$) commutes with $\tilde{\varrho}_i \equiv \varrho_i(\alpha + \delta)$ with δ a small perturbation of the control parameter α , i.e., $[\varrho_i, \tilde{\varrho}_i] = 0$. This commuting property will great facilitate our study of RFS below.

In addition, there is an translational invariance in the Hamiltonian due to the periodic boundary condition, which leads to the fact that any two terms of the form $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ equals to each other. Applying the Feynman-Hellman theorem [26], i.e., $\partial_\alpha E_n = \langle n | \partial_\alpha H | n \rangle$ with $|n\rangle$ the non-degenerate eigenstate of Hamiltonian H and E_n the eigenenergy. To the GS, the spin correlators corresponding to two NN spin pairs are written as

$$\begin{aligned} \langle \sigma_{1z} \sigma_{2z} \rangle &= \frac{8}{3} (e_0 - \alpha \partial_\alpha e_0), \\ \langle \sigma_{2z} \sigma_{3z} \rangle &= \frac{8}{3} \partial_\alpha e_0, \end{aligned} \quad (5)$$

where $e_0 \equiv E_0/N$ represents the GS energy (denoted by E_0) per spin. The above equation gives a direct relation between the spin correlators and the GS energy and its first derivative. In other words, the elements of the RDMs are completely determined by e_0 and $\partial_\alpha e_0$.

B. Reduced fidelity susceptibility

First, we briefly review the definitions of fidelity and fidelity susceptibility. For two pure states $|\Psi(\alpha)\rangle$ and $|\Psi(\alpha + \delta)\rangle$ with δ a small change of the external parameter α , their overlap or *fidelity* is defined as [3]

$$F(\alpha) = |\langle \Psi(\alpha) | \Psi(\alpha + \delta) \rangle|. \quad (6)$$

The extension to the mixed states is in general the *Uhlmann fidelity* [27, 28]

$$F(\alpha) = \text{tr} \sqrt{\rho(\alpha)^{1/2} \rho(\alpha + \delta) \rho(\alpha)^{1/2}}, \quad (7)$$

with $\rho(\alpha)$ and $\rho(\alpha + \delta)$ the two density matrices. The fidelity susceptibility is defined as

$$\chi = \lim_{\delta \rightarrow 0} \frac{-2 \ln F}{\delta^2}. \quad (8)$$

Thus the fidelity susceptibility does not depend on δ .

Then, we will generally calculate the fidelity between two Hermitian and semi-positive definite density matrices $\varrho \equiv \varrho(\alpha)$ and $\tilde{\varrho} \equiv \varrho(\alpha + \delta)$, which are commute with each other, i.e., $[\varrho, \tilde{\varrho}] = 0$, so that they can be diagonalized simultaneously. With the definition of fidelity, we get

$$F_\varrho = \text{tr} \sqrt{\varrho^{1/2} \tilde{\varrho} \varrho^{1/2}} = \sum_i \sqrt{\lambda_i \tilde{\lambda}_i}, \quad (9)$$

where λ_i s and $\tilde{\lambda}_i$ s are the eigenvalues of ϱ and $\tilde{\varrho}$, respectively. Since zero eigenvalues have no contribution to F_ϱ , we only need to consider the nonzero ones. In the following, the subscript i in \sum_i only refers to the nonzero eigenvalues of ϱ .

For a small change δ , $\tilde{\lambda}_i$ can be expanded as $\tilde{\lambda}_i \equiv \lambda(\alpha + \delta) \simeq \lambda_i + (\partial_\alpha \lambda_i) \delta + (\partial_\alpha^2 \lambda_i) \delta^2 / 2 + O(\delta^3)$. Then the fidelity for matrix ϱ becomes

$$F_\varrho = \sum_i \left\{ \lambda_i + \frac{\delta}{2} \partial_\alpha \lambda_i + \frac{\delta^2}{4} \left(\partial_\alpha^2 \lambda_i - \frac{(\partial_\alpha \lambda_i)^2}{2\lambda_i} \right) \right\}. \quad (10)$$

Here we have neglected small terms higher than second order. Since $\sum_i \lambda_i \equiv 1$, we have $\sum_i \partial_\alpha \lambda_i = \sum_i \partial_\alpha^2 \lambda_i = 0$. Thus the fidelity is further reduced to

$$F_\varrho = 1 - \frac{\delta^2}{2} \sum_i \frac{(\partial_\alpha \lambda_i)^2}{4\lambda_i}. \quad (11)$$

Therefore, according to the relation between fidelity and susceptibility, $F = 1 - \chi \delta^2 / 2$, which is equivalent to Eq. (8), the fidelity susceptibility χ_ϱ corresponding to the matrix ϱ is obtained as

$$\chi_\varrho = \sum_i \frac{(\partial_\alpha \lambda_i)^2}{4\lambda_i}. \quad (12)$$

This expression of fidelity susceptibility is valid for any commuting density matrices, and the second power on the right-hand side of the equation will lead to an interesting relation between the RFS and the second derivative of GS energy shown in Eq. (15).

C. Connection to quantum phase transitions

In the dimerized model, as the two-spin RDMs with different parameters commute, Eq. (12) is applicable. By using the expression of the RDM (see Eqs. (2)-(4)), after some calculations, the RFS for the density matrix ρ_{ij} is derived as

$$\begin{aligned} \chi_{ij} &= \frac{4(\partial_\alpha \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle)^2}{(3 + 4\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle)(1 - 4\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle)} \\ &= \frac{3(\partial_\alpha \langle \sigma_{iz} \sigma_{jz} \rangle)^2}{4(1 + \langle \sigma_{iz} \sigma_{jz} \rangle)(1 - 3\langle \sigma_{iz} \sigma_{jz} \rangle)}, \end{aligned} \quad (13)$$

which depends on both the spin correlator $\langle \sigma_{iz} \sigma_{jz} \rangle$ itself and its first derivative. In fact, to ensure the eigenvalues of ϱ_1 and ϱ_2 positive (we do not consider the zero eigenvalues), it is required that

$$\langle \sigma_{iz} \sigma_{jz} \rangle \in (-1, \frac{1}{3}), \quad (14)$$

which subsequently guarantees the susceptibility is non-negative.

Now, substituting Eq. (5) into Eq. (13), one can get another forms for the RFSs χ_{12} and χ_{23} as follows

$$\begin{aligned} \chi_{12} &= \frac{16\alpha^2 (\partial_\alpha^2 e_0)^2}{(3 + 8e_0 - 8\alpha \partial_\alpha e_0)(1 - 8e_0 + 8\alpha \partial_\alpha e_0)}, \\ \chi_{23} &= \frac{16 (\partial_\alpha^2 e_0)^2}{(3 + 8\partial_\alpha e_0)(1 - 8\partial_\alpha e_0)}, \end{aligned} \quad (15)$$

in terms of GS energy and its first and second derivatives.

One key observation is that the numerators of the above two expressions happen to be proportional to the square of the second derivative of GS energy. Since the first derivative of energy is easily to be checked continuous (see Eq. (21)) and the denominators are ensured to be positive and finite by Eq. (14), the singularities of the RFSs are determined only by the numerators. That is, if the second derivative of GS energy is singular at the critical point, the RFSs is singular too. On the other hand, it is known that the divergence of the second derivative of GS energy reflects the second-order QPTs of the system, which is shown in Ref. [12] explicitly as

$$\partial_\alpha^2 e_0 = \sum_{n \neq 0}^N \frac{2|\langle \Psi_n | H_1 | \Psi_0 \rangle|^2}{N(E_0 - E_n)}, \quad (16)$$

where $H_1 = \partial_\alpha H$ is the driving term of the Hamiltonian H , and $|\Psi_n\rangle$ is the eigenvector corresponding to the eigenvalue E_n of H . Eq. (16) shows that the vanishing energy gap in the thermodynamic limit can lead to the singularity of the the second derivative of GS energy. Therefore, both the two-spin RFSs can exactly reflects the second-order QPTs in this model. In addition, the second power in the numerators of the expressions, which origins from the relation obtained in Eq. (12), indicates that the two-spin RFSs is more effective than the second derivative of the GS energy in measuring QPTs. Furthermore, by the fidelity approach, it will be shown in Sec. III that the dimerized AHC has a second-order critical point at $\alpha = 1$.

III. FINITE-SIZE AND CRITICAL BEHAVIOR

In this section, we consider the critical behavior of the 1D spin-1/2 dimerized AHC. It is known that, for $0 < \alpha \ll 1$, the coupling between two dimers is so weak that all the spins are locked into singlet states, while for $\alpha = 1$, the system is reduced to the uniform AHC. Hence, it

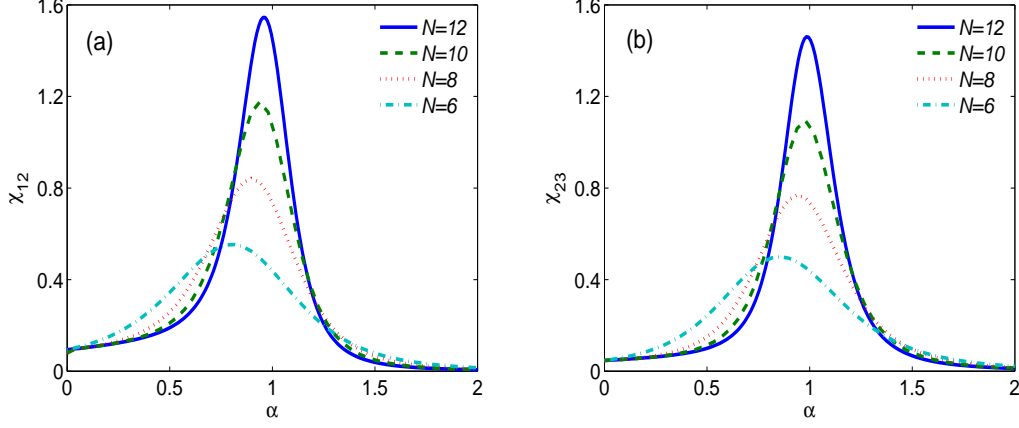


FIG. 1: Reduced fidelity susceptibilities (a) χ_{12} and (b) χ_{23} versus α for $N = 6, 8, 10, 12$ for the dimerized Heisenberg chain.

has already been proved that the dimerized AHC has a critical point at $\alpha = 1$ [21, 22, 23, 24], which exactly exists in the thermodynamic limit $N \rightarrow \infty$.

A. Finite-size behavior

1. Analytical results for $N = 4$ case

For the case that the total spins $N = 4$, the analytical results can be obtained. In this case, the GS energy per spin of the system is [23, 29]

$$e_0 = -\frac{1}{4} \left(\frac{1+\alpha}{2} + \sqrt{1-\alpha+\alpha^2} \right), \quad (17)$$

with its first and second derivatives being

$$\begin{aligned} \partial_\alpha e_0 &= \frac{1}{8} \left(-1 + \frac{1-2\alpha}{\sqrt{1-\alpha+\alpha^2}} \right), \\ \partial_\alpha^2 e_0 &= -\frac{3}{16(1-\alpha+\alpha^2)^{3/2}}. \end{aligned} \quad (18)$$

Then the susceptibilities of the RDMs ρ_{12} and ρ_{23} can be derived from Eq. (15) as

$$\chi_{12} = \chi_{23} = \frac{3}{16(1-\alpha+\alpha^2)^2}. \quad (19)$$

From Eq. (19) we see that χ_{12} and χ_{23} have the same expressions, and there is no singularity over parameter α . However, take derivation of the expression with respect to α , one will find that there is a maximum of χ_{12} (or χ_{23}) at $\alpha = 0.5$, which is also the maximum position of $\partial_\alpha^2 e_0$ as shown in Eq. (18). However, the maximum position $\alpha = 0.5$ deviates from the real critical point $\alpha = 1$ and can be called *pseudo-critical point* due to the finite size of the system. In addition, the different powers in the expressions of χ_{12} (or χ_{23}) and $\partial_\alpha^2 e_0$ over the factor

$(1-\alpha+\alpha^2)$, i.e., the former is $3/2$ and the latter is 2 , shows that the RFS is more sensitive around the critical point.

Besides, the exact equivalence between χ_{12} and χ_{23} is in contract with concurrences as shown in Ref. [23]. There, the concurrences for the reduced system, i.e., C_{12} and C_{23} are unequal to each other and have a crossing point at $\alpha = 1$, which leads to the mean concurrence takes its maximum at the critical point $\alpha = 1$. This is because the concurrences C_{12} and C_{23} are only related to the GS energy and its first derivative over α , respectively. However, the RFSs shown in Eq. (15) are also determined by the second derivative of GS energy, which leads to the identical behavior between χ_{12} and χ_{23} .

2. Numerical results for $N = 6, 8, 10, 12$

For the case that the total spins $N > 4$, we use exact diagonalization method to examine the critical behavior of the system in terms of the RFSs. The results for $N = 6, 8, 10, 12$ are shown in Fig. 1.

It is seen that both the RFSs χ_{12} and χ_{23} can well reflect the critical behavior of the system. With increasing system size, the pseudo-critical point exhibited by χ_{12} (or χ_{23}) approaches to the real critical point $\alpha = 1$. Besides, the larger N becomes, the higher and shaper the peak of χ_{12} (or χ_{23}) is.

It should be noticed that there is a slight difference between χ_{12} and χ_{23} for a given α and N , which results from the difference between the spin correlators shown in Eq. (5). In fact, the two spin correlators are equivalent, if we exchange the two kinds of NN couplings. Thus χ_{12} and χ_{23} are also equivalent in identifying QPTs.

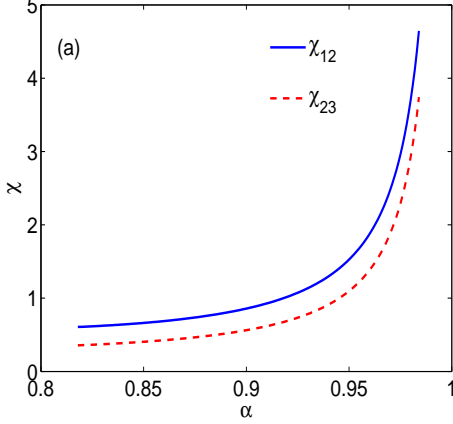


FIG. 2: Reduced fidelity susceptibilities versus α in the thermodynamic limit for the dimerized Heisenberg chain, with $c = 0.3891$ and the exponent $p = 1.4417$ over the range of $0.001 \leq \eta \leq 0.1$ [33], i.e., $0.8182 \leq \alpha \leq 0.9880$.

B. Infinite-size critical behavior

Now, we consider the thermodynamic limit. To be consistent with the former works, we adopt a new parameter $\eta \equiv (1 - \alpha)/(1 + \alpha)$. When the system approaches to the uniform chain limit, i.e., $\eta \rightarrow 0$, analytical studies obtained by renormalization group [30, 31] had predicted that the GS energy per spin e_0 should diverge as a power law times a logarithmic correction, i.e., $\eta^{4/3}/|\ln \eta|$. However, it is restricted to an extremely small range $\eta < 0.02$ [22]. Thereafter, some numerical results pointed out that a pure power-law behavior is reasonably simple and accurate for larger η as well [22, 32, 33].

For generality, we assume a power law of e_0 as the

form $c\eta^p$ with c an overall constant. The exponent p are given differently over different η ranges. Hitherto, almost all the works [22, 32, 33] show that $1 < p < 2$ over the range $0 < \eta < 1$. For example, using the DMRG approach, in [22], the exponent is fit to be $p = 1.45$ over the range of $0.008 \lesssim \eta \lesssim 0.1$ with $c = 0.39$, and in Ref. [33], it is estimated in the range of $0.001 \leq \eta \leq 0.1$ as that $p = 1.4417$ with $c = 0.3891$. Thus we will restrict $1 < p < 2$ in the following. The GS energy per spin in the thermodynamic limit can be written accordingly as [22]

$$e_0(\eta) = \frac{1}{1 + \eta}(e_0(0) - c\eta^p), \quad (20)$$

where $e_0(0) = 1/4 - \ln 2$ is the GS energy per spin for $\eta = 0$.

The above expression shows that the GS energy follows the power law behavior η^p . This gives a prediction of the critical point of the RFSs. From Eq. (20), we can easily get the first and second derivatives of GS energy per spin in the thermodynamic limit as

$$\begin{aligned} \partial_\alpha e_0 &= \frac{c}{2}(2p + \alpha - 1)(1 + \alpha)^{-1}(1 - \alpha)^{p-1}, \\ \partial_\alpha^2 e_0 &= -2c(p - 1)p(1 + \alpha)^{-(p+1)}(1 - \alpha)^{p-2}. \end{aligned} \quad (21)$$

It is seen that, as $\alpha > 0$ and $1 < p < 2$, the first derivative of e_0 does not diverge for any allowed α value, while the second derivative of e_0 has a singular point $\alpha = 1$. According to Eq. (15), it is no doubt that the RFSs also diverges at $\alpha = 1$. That is, the dimerized AHC has a second-order critical point $\alpha = 1$.

Next we discuss the critical behavior of the RFSs around the critical point. Insert Eq. (21) into Eq. (15), we obtain the RFSs as

$$\begin{aligned} \chi_{12} &= -\frac{c^2 p^2 (p - 1)^2 \eta^{-2+2p} (\eta - 1)^2 (\eta + 1)^4}{16 \left[c^2 (p + \eta - p\eta)^2 \eta^{2p} + c(2 \ln 2 - 1)(p + \eta - p\eta) \eta^{1+p} + \ln 2 (\ln 2 - 1) \eta^2 \right]}, \\ \chi_{23} &= -\frac{c^2 p^2 (p - 1)^2 \eta^{-2+2p} (\eta + 1)^6}{16 \left[c^2 (p - \eta + p\eta)^2 \eta^{2p} - c(2 \ln 2 - 1)(p - \eta + p\eta) \eta^{1+p} + \ln 2 (\ln 2 - 1) \eta^2 \right]}. \end{aligned} \quad (22)$$

When $\alpha \rightarrow 1$, i.e., $\eta \rightarrow 0$, we only consider the leading terms in the expressions and get the critical behavior of the RFSs as

$$\chi_{12}, \chi_{23} \sim \eta^{2p-4} \sim (1 - \alpha)^{2p-4}. \quad (23)$$

Obviously, for $1 < p < 2$, both of them diverge at $\eta = 0$, i.e., $\alpha = 1$, as displayed in Fig. 2. It is shown that the two RFSs diverge quickly when α approaches to 1. For a given α , χ_{12} and χ_{23} are remarkably larger than

those in the finite-size cases. In addition, the different power between $\partial_\alpha^2 e_0$ and $\chi_{12}(\chi_{23})$ over the factor $(1 - \alpha)$ indicates that these RFSs are more singular around the critical point.

IV. GENERAL CONNECTION BETWEEN REDUCED FIDELITY AND QUANTUM PHASE TRANSITIONS

A. More exemplifications

In the above, we have illustrated the connection between RFS and QPTs in the spin-1/2 dimerized AHC, which has SU(2) symmetry. Actually, it is straightforward that the RFS expression (13) is general for an arbitrary spin-1/2 Hamiltonian with SU(2) symmetry. Combined with the translation symmetry, it is easy to obtain a relation between RFS and QPTs like Eq. (15). In the following, we would like to give another two exemplifications, which are also of SU(2) and translation symmetries. One is the mixed-spin (1/2, S) dimerized Heisenberg chain with S an arbitrary spin length, the other one is the spin-1 bilinear-biquadratic model.

The Hamiltonian for the mixed-spin dimerized Heisenberg chain with alternated spins \mathbf{S}_1 and \mathbf{S}_2 is

$$H_F = \sum_{i=1}^{N/2} (\mathbf{S}_{1,i} \cdot \mathbf{S}_{2,i} + \alpha \mathbf{S}_{2,i} \cdot \mathbf{S}_{1,i+1}), \quad (24)$$

here, \mathbf{S}_1 and \mathbf{S}_2 denote the spin-1/2 and spin- S operators respectively, and α is the ratio between the two kinds of NN spin couplings. The periodic boundary condition is assumed. As the system is of SU(2) symmetry, the RDM between two NN coupling spins can be expressed in the coupled angular momentum representation as [34]

$$\begin{aligned} \rho_{ij} = & \frac{F}{2S} \sum_{J_z=-S+1/2}^{S-1/2} |S-1/2, J_z\rangle \langle S-1/2, J_z| \\ & + \frac{1-F}{2S+2} \sum_{J_z=-S-1/2}^{S+1/2} |S+1/2, J_z\rangle \langle S+1/2, J_z|, \end{aligned} \quad (25)$$

with J_z the total spin along the z direction of the two spins and $F = (S - 2\langle \mathbf{S}_{1,i} \cdot \mathbf{S}_{2,j} \rangle) / (2S + 1)$. Since ρ_{ij} is diagonal, the RFS expression (12) is available. Then

$$\chi_{ij} = \frac{(\partial_\alpha \langle \mathbf{S}_{1,i} \cdot \mathbf{S}_{2,j} \rangle)^2}{(S - 2\langle \mathbf{S}_{1,i} \cdot \mathbf{S}_{2,j} \rangle)(S + 1 + 2\langle \mathbf{S}_{1,i} \cdot \mathbf{S}_{2,j} \rangle)}. \quad (26)$$

Meanwhile, the system is translational invariant. Thus applying the Feynman-Hellman theorem to the GS of the system, we get the expressions for the two kinds of RFSs between two NN spin pairs

$$\begin{aligned} \chi_{12} &= \frac{4\alpha^2 (\partial_\alpha^2 e_0)^2}{(S - 4e_0 + 4\alpha \partial_\alpha e_0)(S + 1 + 4e_0 - 4\alpha \partial_\alpha e_0)}, \\ \chi_{23} &= \frac{4 (\partial_\alpha^2 e_0)^2}{(S - 4\partial_\alpha e_0)(S + 1 + 4\partial_\alpha e_0)}. \end{aligned} \quad (27)$$

Obviously, when $S = 1/2$, the above expression reduces to Eq. (15). The two RFSs is proportional to the second derivative of the GS energy per spin $e_0 \equiv e_0(\alpha)$. That is, the RFS also has the possibility to signal the second-order QPTs of a mixed-spin system.

Furthermore, the general expression of RFS (13) could also be extended to high-spin system, like the spin-1 bilinear-biquadratic model, which describes the structure of some materials, such as LiVGe₂O₆[37, 38]. The Hamiltonian reads

$$H_{BB} = \sum_{i=1}^N [\cos \theta (\mathbf{S}_i \cdot \mathbf{S}_{i+1}) + \sin \theta (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2], \quad (28)$$

here \mathbf{S}_i denotes the spin-1 operator, and θ reflects the different coupling strengths. The periodic boundary condition is assumed as well. Obviously, this Hamiltonian is also of SU(2) and translation symmetries. In Eq. (24) of Ref. [35], the QPT of this model is studied by using the RFS between NN-coupling spins, which happens to be proportional to the second derivative of the GS energy density $e_0 \equiv e_0(\theta)$, i.e.,

$$\chi_{12} \propto (e_0 + \partial_\theta^2 e_0)^2. \quad (29)$$

This further confirms that the two-spin RFS is an effective tool to reveal the second-order QPTs even for high-spin systems.

All the above results show that the two-spin RFS is tied to the corresponding spin-correlator, while the latter is related to the GS energy through Feynman-Hellman theorem. Then the RFS is connected to the square of the second derivative of the GS energy, which is used to characterize the second-order QPTs, as shown in Eqs. (15), (27), (29). Moreover, the square relation between the two-body RFS and the second derivative of GS energy Eq. (15) holds for a broad class of systems with SU(2) and translation symmetries, and thus the RFS might be more sensitive than... the second derivative of the GS energy in characterizing QPTs.

B. General connection between reduced fidelity and quantum phase transitions

The models considered above are all of SU(2) and translation symmetries. It is noticed that the definition of RF (7) depends only on the RDM, which may contains sufficient information about QPTs. This inspires us to infer that for a more general case, QPTs are essentially related to the RDM. In [39], they have provided a powerful substantiation. They demonstrated that, under certain general conditions, the elements of two-body RDM are able to signal the QPTs. They consider a general Hamiltonian that contains two-body interaction like

$$H = \sum_{i\alpha\beta} \epsilon_{\alpha\beta}^i |\alpha_i\rangle \langle \beta_i| + \sum_{ij\alpha\beta\gamma\kappa} V_{\alpha\beta\gamma\kappa}^{ij} |\alpha_i\rangle |\beta_j\rangle \langle \gamma_i| \langle \kappa_j|, \quad (30)$$

where i, j enumerate N particles and $\{|\alpha_i\rangle\}$ is a basis for the Hilbert space. For the nondegenerate GS $|\psi\rangle$, its GS energy is $E_0 = \langle\psi|H|\psi\rangle$, and the element of the corresponding two-particle RDM is $\rho_{\gamma\delta\alpha\beta}^{ij} = \langle\psi|\alpha_i\beta_j\rangle\langle\gamma_i\delta_j|\psi\rangle$. Thus the relation between energy and RDM is $E_0 = \sum_{ij} \text{tr}[U(ij)\rho^{ij}]$, where $U_{\alpha\beta\gamma\kappa}(ij) = \epsilon_{\alpha\gamma}^i \delta_{\beta\kappa}^j / N_i + V_{\alpha\beta\gamma\kappa}^{ij}$ with N_i the number of particles that particle i interacts with and $\delta_{\beta\kappa}^j$ the Kronecker symbols on particle j . Then using the Feynman-Hellman theorem, the derivatives of energy per particle ($e_0 \equiv E_0/N$) are obtained as

$$\partial_\xi e_0 = \frac{1}{N} \sum_{ij} \text{tr}[(\partial_\xi U(ij))\rho_{ij}], \quad (31)$$

$$\begin{aligned} \partial_\xi^2 e_0 = \frac{1}{N} \sum_{ij} \{ & \text{tr}[(\partial_\xi^2 U(ij))\rho_{ij}] \\ & + \text{tr}[(\partial_\xi U(ij))\partial_\xi \rho_{ij}] \}, \end{aligned} \quad (32)$$

where it follows from Eq. (31) that $\sum_{ij} \text{tr}[U(ij)(\partial_\xi \rho_{ij})] = 0$. As is known, according to the classical definition of phase transitions given in terms of the free energy [40], in the limit of $T = 0$, a first-order QPT (second-order QPT) is characterized by a discontinuity in the first (second) derivative of the GS energy (see also Eq. (16)). Therefore, if $U(ij)$ is a smooth function of the Hamiltonian parameter ξ , the origin of first-order QPTs is due to the discontinuity of one or more of the ρ_{ij} 's at the critical point according to Eq. (31). Whereas, if ρ_{ij} is finite at the critical point, the origin of second-order QPTs is the fact one or more of the $\partial_\alpha \rho_{ij}$'s diverge at the critical point.

Based on these facts, one find that if $U(ij)$ is a smooth function and the first derivative of the elements of ρ_{ij} diverges at the critical point, then $\partial_\xi^2 e_0$ diverges too, which indicates a second-order QPT. For example, in our models considered, the elements of ρ_{ij} are decided by $\langle\sigma_{iz}\sigma_{jz}\rangle$, which is connected to $\partial_\xi e_0$ via Feynman-Hellman theorem. Thus the relation revealed by Eq. (32) may be the origin of the relation between RFS and QPTs. This is not restricted to the systems with SU(2) invariance, and a more explicit and direct relation between RFS and QPTs may need further deep considerations.

In addition, the relation between the reduced fidelity (denoted as F_R) and its corresponding global fidelity F_G is given already as $F_G \leq F_R$ [41]. According to relation (8), the corresponding susceptibilities satisfy $\chi_G \geq \chi_R$. However, all the previous works [14, 15, 16, 17, 18, 19] and this work confirm that the reduced fidelity approach is as effective as global fidelity in characterizing QPTs,

and in some cases, such as the models mentioned above, it is only necessary to know the GS energy of system in calculating the RFS, rather than its GS for the global fidelity, which is generally not easy to be obtained.

V. CONCLUSION

In conclusion, we have studied the critical behavior of the 1D spin-1/2 antiferromagnetic Heisenberg chain with dimerization in terms of RFS. For the GS of the system, two kinds of RFSs between two NN spin pairs are considered. It is interesting that, due to the SU(2) and translation symmetries, the singularities of these RFSs are just determined by the square of the second derivative of the GS energy, which means the RFS is more effective than the second derivative of the GS energy in identifying the second-order QPTs. Explicit calculations are also carried out both in finite-size and infinite-size situations. It is found that, as the system size increases, the pseudo-critical points of the RFSs approach to the real critical point $\alpha = 1$. In the thermodynamic limit, we give the critical exponent of the two RFSs. These results further convince us that the critical behavior of the system can be reflected by the fidelity of its two-spin subsystem, which is of practical use in experiments.

Furthermore, concluding the results obtained in the spin-1/2 dimerized model, we examine another two examples, i.e., the mixed-spin dimerized Heisenberg chain and the spin-1 bilinear-biquadratic model, which have the SU(2) and translation symmetries as well. It is also found that the RFSs are directly connected to the square of the second derivative of the GS energy, which indicates that for a broad class of systems with SU(2) and translation symmetries, the RFS is more effective than the second derivative of the GS energy in reflecting second-order QPTs. Moreover, the origin between RFS and QPTs is found to be generally rooted in the relations between the elements of the RDM and derivatives of GS energy, which provides a general proof for the fact that RFS can be used to detect the second-order QPTs of the system.

Acknowledgements This work was supported by the Program for New Century Excellent Talents in University (NCET), the NSFC with grant No. 90503003, the State Key Program for Basic Research of China with grant No. 2006CB921206, the Specialized Research Fund for the Doctoral Program of Higher Education with grant No. 20050335087.

-
- [1] S. Sachdev, Quantum Phase Transitions (Cambridge University Press, England, 1999).
 - [2] H. T. Quan, Z. Song, X. F. Liu, P. Zanardi, and C. P. Sun, Phys. Rev. Lett. **96**, 140604 (2006).
 - [3] P. Zanardi and N. Paunković, Phys. Rev. E **74**, 031123

(2006).

- [4] W. L. You, Y. W. Li, and S. J. Gu, Phys. Rev. E **76**, 022101 (2007).
- [5] P. Zanardi, P. Giorda, and M. Cozzini, Phys. Rev. Lett., **99**, 100603 (2007).

- [6] M. F. Yang, Phys. Rev. B **76**, 180403(R) (2007).
- [7] P. Buonsante and A. Vezzani, Phys. Rev. Lett **98**, 110601 (2007).
- [8] L. Campos Venuti, M. Cozzini, P. Buonsante, F. Massel, N. Bray-Ali, and P. Zanardi, Phys. Rev. B **78**, 115410 (2008).
- [9] S. Chen, L. Wang, S. J. Gu, and Y. Wang, Phys. Rev. E **76**, 061108 (2007).
- [10] S. Yang, S. J. Gu, C. P. Sun and H. Q. Lin, Phys. Rev. A **78**, 012304 (2008).
- [11] L. Gong and P. Tong, Phys. Rev. B **78**, 115114 (2008).
- [12] S. Chen, L. Wang, Y. Hao, and Y. Wang,
- [13] W. L. You, Y. W. Li, and S. J. Gu, Phys. Rev. E **76**, 022101 (2007).
- [14] H. Q. Zhou, Roman Orús and G. Vidal, Phys. Rev. Lett. **100**, 080601 (2008).
- [15] H. Q. Zhou, arXiv:0704.2945.
- [16] N. Paunković, P. D. Sacramento, P. Nogueira, V. R. Vieira, and V. K. Dugaev, Phys. Rev. A **77**, 052302 (2008).
- [17] H. M. Kwok, W. Q. Ning, S. J. Gu, and H. Q. Lin, Phys. Rev. E **78**, 032103 (2008).
- [18] J. Ma, L. Xu, H. N. Xiong, and X. Wang, arXiv:0805.4062.
- [19] J. Ma, L. Xu, and X. Wang, arXiv:0808.1816.
- [20] P. L. Nordio, Z. G. Soos, and H. M. McConnell, Annu. Rev. Phys. Chem. **17**, 237 (1966).
- [21] K. P. Schmidt and G. S. Uhrig, Phys. Rev. Lett. **90**, 227204 (2003).
- [22] T. Papenbrock, T. Barnes, D. J. Dean, M. V. Stoitsov, and M. R. Strayer, Phys. Rev. B **68**, 024416 (2003).
- [23] Z. Sun, X. Wang, A. Z. Hu, and Y. Q. Li, Commun. Theor. Phys. **43** 1033 (2005).
- [24] Y. Chen, P. Zanardi, Z. D. Wang, and F. C. Zhang, New J. Phys. **8** 97 (2006).
- [25] X. Wang and P. Zanardi, Phys. Lett. A **301**, 1 (2002).
- [26] L. D. Landau and E. M. Lifshitz, Quantum Mechanics—Non-relativistic Theory, Course of Theoretical Physics, Vol. 3, 3rd ed. (Pergamon, Oxford, 1977), Sec. 11.
- [27] A. Uhlmann, Rep. Math. Phys. **9**, 273 (1976).
- [28] R. Jozsa, J. Mod. Opt. **41**, 2315 (1994).
- [29] X. Hao and S. Zhu, arXiv:0803.0770.
- [30] M. C. Cross and D. S. Fisher, Phys. Rev. B **19**, 402 (1979).
- [31] J. L. Black and V. J. Emery, Phys. Rev. B **23**, 429 (1981).
- [32] T. Barnes, J. Riera, and D. A. Tennant, Phys. Rev. B **59**, 11384 (1999).
- [33] M. Kumar, S. Ramasesha, D. Sen, and Z. G. Soos, Phys. Rev. B **75**, 052404 (2007).
- [34] J. Schliemann, Phys. Rev. A, **68**, 012309 (2003).
- [35] X. Wang and S. J. Gu, arXiv:0809.4898.
- [36] F. D. M. Haldane, Phys. Lett. A **93**, 464 (1983), and Phys. Rev. Lett. **50**, 1153 (1983), and J. Appl. Phys. **57**, 3359 (1985).
- [37] P. Millet, F. Mila, F. C. Zhang, M. Mambrini, A. B. Van Oosten, V. A. Pashchenko, A. Sulpice, and A. Stepanov, Phys. Rev. Lett. **83**, 4176 (1999).
- [38] J. Lou, T. Xiang, and Z. Su, *ibid*, **85**, 2380 (2000).
- [39] L. A. Wu, M. S. Sarandy, and D. A. Lidar, Phys. Rev. Lett. **93**, 250404 (2004).
- [40] L. E. Reichl, A Modern Course in Statistical Physics (John Wiley and Sons, New York, 1998).
- [41] M. A. Nielsen and I. L. Change, Quantum Computation and Quantum Information (Cambridge University Press, Cambridge, U.K., 2000).